Development of an Integrated Modeling Framework for Simulations of Coastal Processes in Deltaic Environments Using High-Performance Computing

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LONG-TERM GOALS

The long-term goal of our project is to develop and enhance research and educational capabilities in the area of coastal engineering and science at Louisiana State University (LSU) while simultaneously supporting the Navy's research goals in the area of Coastal Geosciences. The focus of the present work is to develop a new modeling framework for simulations of coastal processes in deltaic environments using advanced numerical methods and high performance computing technology. In particular, the utilization of adaptive numerical methods such as the spectral element method on modern computer platforms with thousands of multi-core processors will enable coastal modelers to simulate complex physical processes with improved accuracy and efficiency.

[1] Dynamics of Potential Vorticity in the Swash and Surf Zones, PI: Q. Jim Chen

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OBJECTIVES

The specific objectives of this project are to:

- Develop the capability of modeling coastal circulation and nearshore surface waves in deltaic sedimentary and hydrodynamic environments in an integrated modeling framework by extending the Boussinesq theory for nearshore hydrodynamics to muddy coasts and non-hydrostatic three-dimensional (3D) flow regimes with stratifications.
- Complement the Office of Naval Research recent research initiatives on Tidal Flats and Wave-Mud Interactions by integrating the new modeling system with the field data collected in those programs.
- Simulate large-scale, long-term problems in the deltaic environment by integrating the application-oriented modeling system with massive-processor computing facilities and technologies available at LSU and in Louisiana.
- Quantify the generation, transport and dissipation of potential vorticity in the surf and swash zones, as well as the momentum exchange between the two dynamical regions.

APPROACH

The research project consists of theoretical formulation and analysis, the development and verification of an advanced modeling system using the spectral/hp element methods and high-performance computing technologies, and the utilization of the new model as a research tool to advance knowledge and understanding of coastal circulation and nearshore waves in deltaic sedimentary and hydrodynamic environments. Relevant methodologies in three disciplines: civil engineering, physical oceanography and computational science, are being utilized. Interdisciplinary interactions are taking place among the investigators in different fields and through recruiting graduate students from the three disciplines. All project members meet together weekly, with meetings alternating between focusing on coastal science and computational science. Code development and document preparation is enabled through a project-wide source code versioning system.

A new approach is taken to meet the objectives of this project: 1) Use the Boussinesq theory to improve the efficiency of non-hydrostatic 3D Navier-Stokes equation solvers as well as to extend the applicability of the modeling system to deltaic environments, and 2) utilize spectral/hp element methods with unstructured grids to solve the partial differential equations (PDE) under realistic deltaic conditions on high-performance, massive-processor computers available at LSU.

The theoretical derivation follows closely the approach of Dalrymple and Liu (1978) for the treatment of soft mud, and the procedure of Chen et al. (2003) and Chen (2006) for

the treatment of surface waves. The Boussinesq approach is not just limited to the modeling of nonlinear surface waves and breaking-generated currents over porous or muddy seabed. An efficient hydrodynamic model for density-stratified flow with a free-surface in the weakly non-hydrostatic regime has been developed by Shen (2001) and Shen and Evans (2004). This formulation allows for applying the weakly non-hydrostatic approximation, similar to the Boussinesq approach to nonlinear surface gravity waves, to strongly nonlinear internal waves in the coastal ocean where the horizontal scale of the density-stratified wave/current motion exceeds the local water depth. The approximation eliminates the vertical dimension of the elliptic equation that is normally required for the fully non-hydrostatic modeling, and as a result the model's computation efficiency is greatly increased by a factor proportional to the number of grid points used for vertical resolution.

The shallow water equations (SWE) are a set of non-linear hyperbolic equations. As the equations are derived under the assumption of hydrostatic pressure, the SWE are only valid for long waves. The source terms can contain forcing due to e.g. bathymetry, bottom friction, atmospheric pressure, Coriolis force, wind stresses and diffusion. As the first step of model developments, we have focused on the homogenous version of the SWE to assess the performance of the computational core. Boussinesq-type models for wave-driven currents are computationally demanding. Taking seabed conditions into account by the new Boussinesq model will further increase the computational effort by a factor of two. It is therefore desired to speed up Boussinesq models for practical applications, in particular for morphological and ecological simulations. The solution to the growing demand of computing power by Boussinesq coastal models is the use of high-performance computing (HPC) technologies.

WORK COMPLETED

Figure 1 illustrates the implementation strategy for the discontinuous Galerkin scheme using the open-source spectral/*hp* library Nektar++ (www.nektar.info). Through Nektar++, the fundamental routines associated with a high-order finite-element method are easily accessible. With regard to the high-order discretizations, our work has been directed towards implementing a solver specific to time-dependent problems. This includes a SWE class containing functions for the evaluation of the flux vectors, numerical fluxes, equation dependent boundary conditions, various source terms, etc. This class provides a SWE solver library.

Our approach in parallelizing the SWE solver was to integrate our code into the Cactus computational framework and provide parallelism through a Cactus "Driver" module (or "thorn'') (see Fig. 1). Cactus (www.cactuscode.org) is an open source problem solving environment designed for scientists and engineers. Its modular structure easily enables parallel computation across different architectures and collaborative code development between different groups. Cactus originated in the academic research community, where it was developed and used over many years by a large international collaboration of physicists and computational scientists.

In order to integrate the serial SWE solver into Cactus, several thorns have been developed. Most importantly, we have designed a “Nektar++” thorn that initializes and populates the data structures of Nektar++. We also provide a “SWE” thorn that contains the actual SWE solver based on routines defined in the SWE solver library.

Integrating the SWE solver in Cactus provides easy access to a maintainable parallel layer that has been developed to support unstructured meshes. The parallel layer is a special module or “thorn” in Cactus referred to as the unstructured mesh driver (UMDriver). This separation of programming tasks enables coastal engineers to focus on developing coastal modeling code using Nektar++ and the computational scientists to focus on parallelism and performance of the unstructured mesh driver.

The unstructured mesh driver utilizes the Zoltan (www.cs.sandia.gov/Zoltan/) library to perform part of its parallel operations such as mesh partitioning and load balancing. The Zoltan library contains a number of tools that simplify the development and improve the performance of parallel, unstructured and adaptive applications. The library is organized as a toolkit, so that application developers can use as little or as much of the library as desired. As the driver layer matures, it will be less dependent on external packages and will be performing many other tasks that are being added, such as support for adaptive mesh refinement, a hyper-slabbing interface and dynamic load balancing.

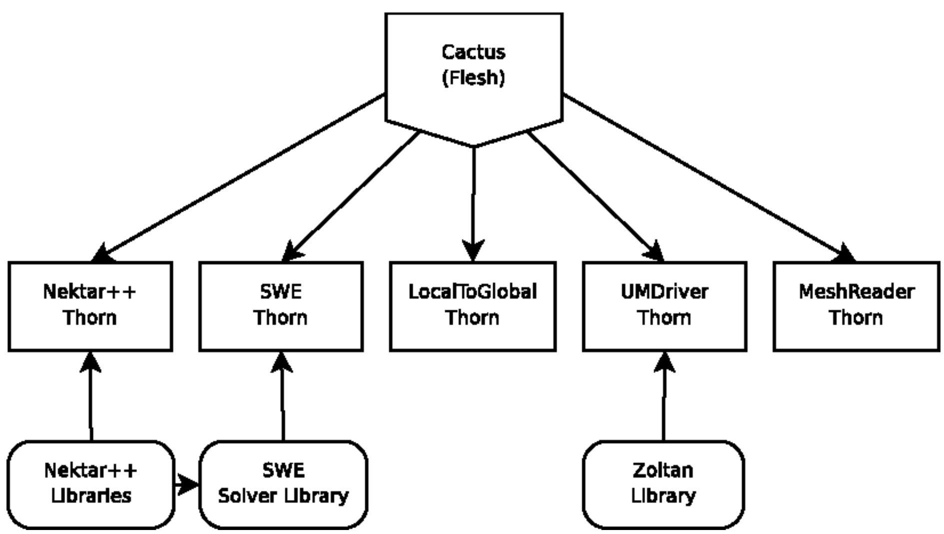

Figure 1: Schematic diagram for the Cactus and Nektar++ interface.

RESULTS

The major results obtained so far are: 1) the implementation of a new SWE solver based on the discontinuous Galerkin spectral/hp element method in Nektar++ interfacing with the Cactus Framework to handle the parallel computing issues, 2) the scaling tests on unstructured meshes for the coupled software, 3) the simulations of wave interaction with five upright cylinders as a testing case, and 4) the implementation of the Boussinesq

model (FUNWAVE) for waves and currents on a solid bed into the Cactus Framework using finite-difference schemes to serve as a verification tool.

To demonstrate a few capabilities and features of the coupled Cactus-Nektar++ software implementation of SWE, some preliminary results of numerical convergence test are presented in Fig. 2. Consider the simple case of a linear standing wave with a wavelength of 10 m in a square 10 m by 10 m basin. The still water depth is 0.5 m. In order to compare with the analytical solution here, we use the linearized SWE. The solution for one wave period was obtained using numerical integration on 10,000 time steps. Figure 2 shows the error and order of convergence measured in the L_2 norm.

***Exponential Convergence Results*:** Spectral/hp element methods provide dual paths to convergence: *p*-refinement and *h*-refinement. Here *p*-refinment refers to the increase in polynomial order of the basis functions for the elements, while *h*-refinement refers to the decreasing mesh size or increasing element numbers and nodes. The key feature of spectral/hp elements is that *p*-refinement gives rise to exponentially fast convergence, as illustrated in Fig. 2 for the standing wave case. It is seen that the numerical errors decrease exponentially before reaching the plateau, as the order of the basis functions increases.

In order to assess the parallel performance of the developed software on multi-processor systems, we need to carry out two types of scaling tests: Weak scaling test and strong scaling test. In weak scaling tests, the computational work per processor (or core) is maintained constant and the total size of the problem increases with increase in number of processors. For an ideal weak scaling, the time to the solution should not increase significantly when the problem size is increased in proportion to the number of processors. On the other hand, strong scaling test uses a fixed problem size and determines the time to solution while increasing the number of processors. For an ideal strong scaling, the time to solution should continue to decrease for a fixed computational work with increasing number of processors. All these tests were performed on the "QueenBee" supercomputer (www.loni.org) that has 680 nodes with each node having 2 quad-core processor (i.e. 8 cores) with 8 Gb RAM.

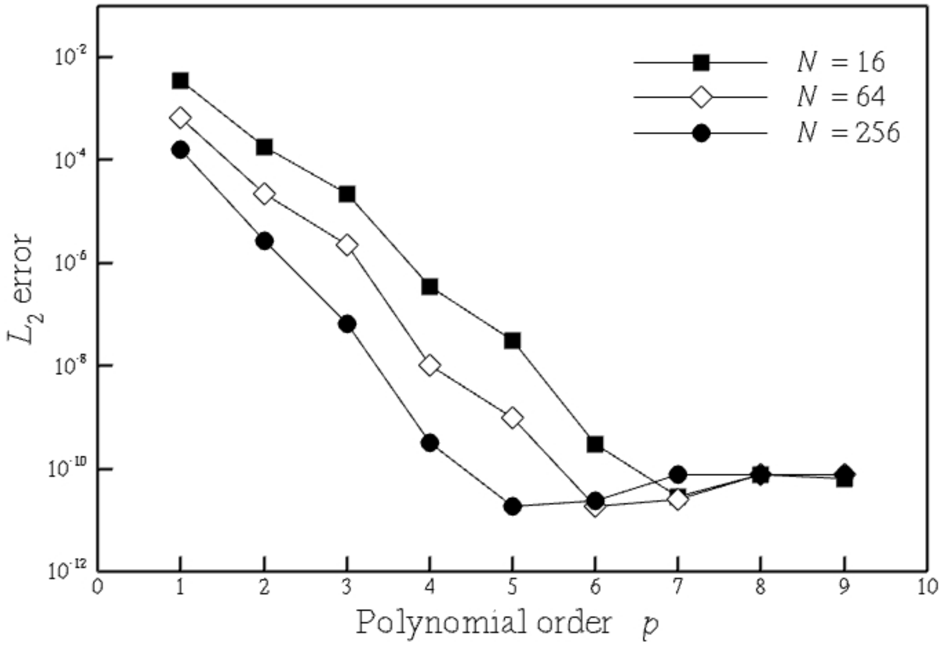

Figure 2: Illustration of exponential convergence

***Weak Scaling Results*:** Tests have been carried out for two types of meshes: consisting of 100 and 900 quadrilaterals per core, respectively. Both sets are run with three different polynomial orders: p = 4, 6 and 8. Thus, the largest run contains 218,700 unique degrees of freedom per core, or a total of roughly 28 million degrees of freedom. Total execution time as well as solution time for the model is recorded for one hundred time steps. Figure 3 (top) shows the solution times (without I/O, initializing and partitioning of the mesh) for 900 quadrilaterals per core mesh. The results from the 100-quaddrilateral-elements-per-core mesh were as expected and hence, are not shown here for the sake of brevity.

We notice that the total wall clock time to completion for all polynomial orders increases as we increase the number of processors and correspondingly the size of the modeling domain (i.e. a weak- scaling test). The parallelization efficiencies range from 95% to 78%, as the number of cores increase from 2 to 128. Additional efforts will be made to further improve the scalability and performance by redesigning the problem setup routines and mesh partitioning routines in the next round of code refinement and optimization.

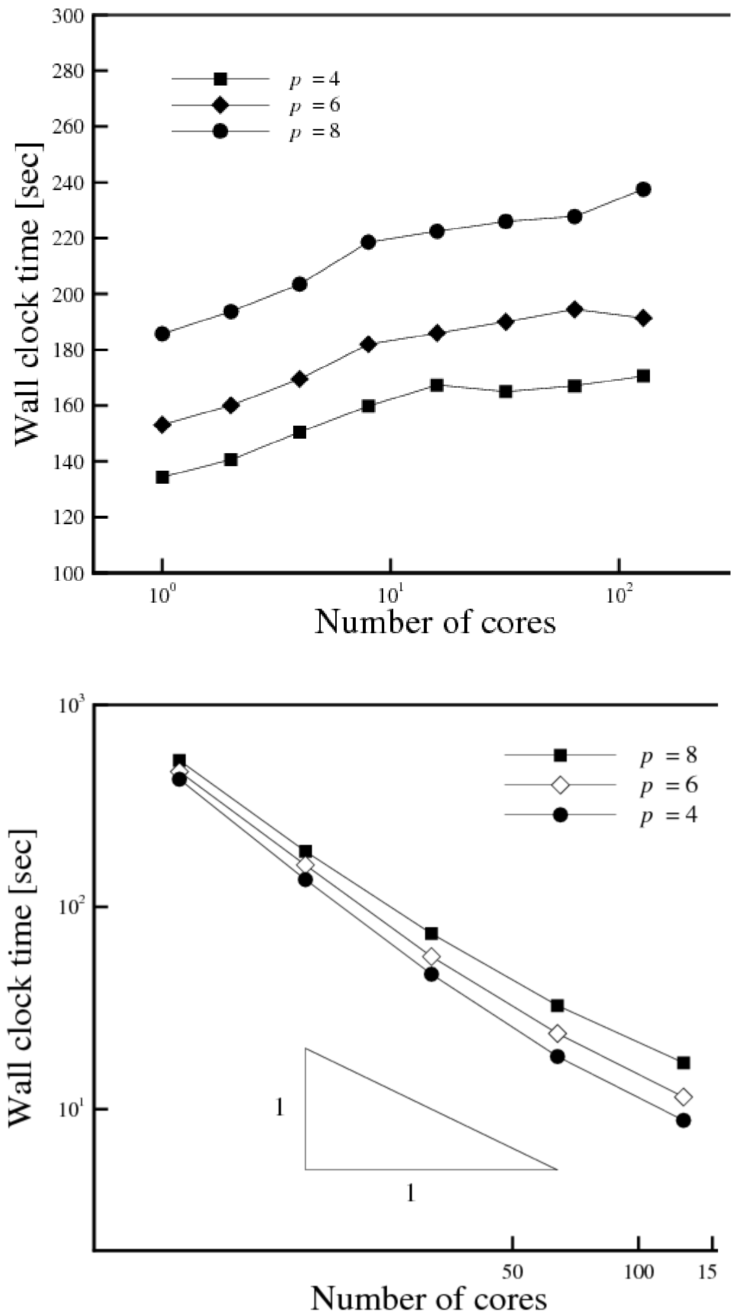

Figure3: Parallel performance: Weak Scaling (top) and Strong Scaling (bottom).

Strong Scaling Results: The final computational load for 128 processors is about 100 elements per core and for the single node (or 8 cores) it translates to 1600 elements per node. Figure 3 (bottom) shows the reduction in solution time for a fixed size problem as the number of processors increased. Various tests have been conducted by changing the polynomial order while keeping the same underlying geometric mesh. Although there is a slight reduction in parallelization efficiency between 64 to 128 cores, these results are highly encouraging from the perspective that now coastal scientists can easily run their

existing single-processor simulations on several hundreds of processors to reduce the total computational time and solve practical problems in an efficient fashion.

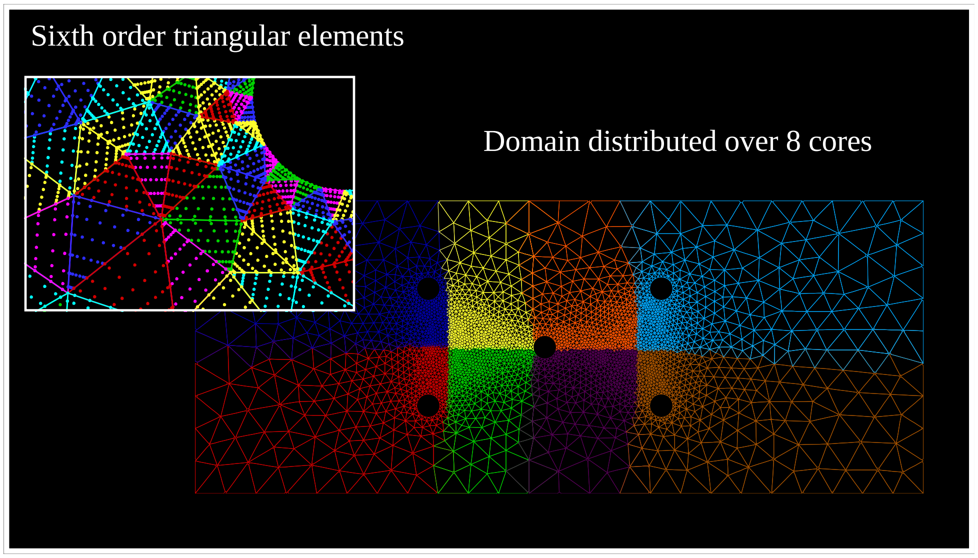

Figure 4: Unstructured triangular element mesh around five cylinders showing the details of collocation points in the interior of the elements for sixth order basis functions. Different colors illustrate the domain decomposition with each color representing the partitioned mesh belonging to each processor.

***Wave Interaction with Five Upright Cylinders*:** As a numerical example to illustrate the sanity of flow physics that is being simulated, wave propagation and interaction with five upright cylinders are simulated. This example has enough complexity to be relevant and yet simple enough to use it for debugging purposes. Figure 4 shows the domain decomposition of an unstructured mesh as well as the details of collocation points inside the spectral elements (inset). Unstructured meshes can easily adapt to complicated features: geometric and/or flow using the *h/p* refinement ability of the spectral element method. As a sample result, computed free surface elevations are presented at two different time instants in Figure 5. It is seen that wave runup on the cylinders as well as wave scattering and diffraction by the group of cylinders are well reproduced by the parallel code.

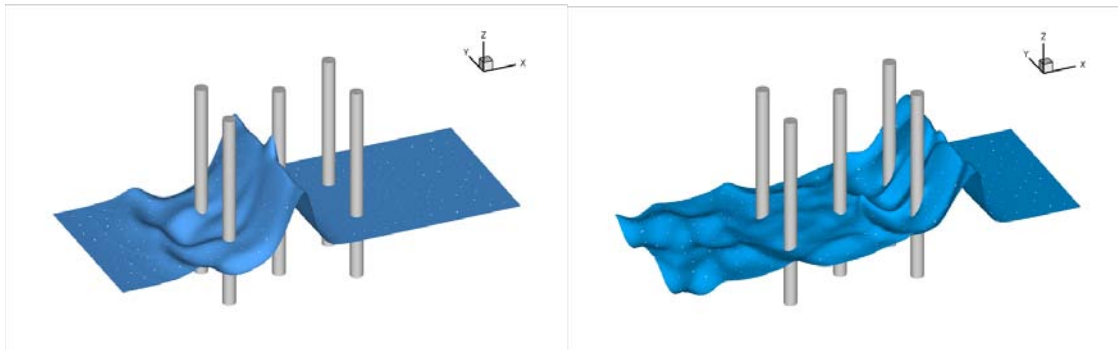

Figure 5: Modeled free surface interacting with five cylinders. Left: t=9.9sec, right: t=20sec.

IMPACT/APPLICATIONS

We have successfully implemented a spectral/*hp* discontinuous Galerkin method for solving the SWE and interfaced it with the Cactus computational framework. We have obtained encouraging results in terms of parallel performance and the coupled software's scaling ability. There are still some unresolved issues in terms of reducing the overheads associated with ghost elements for communication between sub-domains. The use of Cactus provides a path for extensibility, integrating with cutting edge computational hardware and cyberinfrastructure, and building a comprehensive toolkit for coastal applications. We have also demonstrated the relevance of simulated flow physics to the coastal modeling community.

The research is expected to improve the Navy's capability of modeling nearshore surface waves and coastal processes in heterogeneous sedimentary environments. First, the study will extend the applicability of Boussinesq models (Chen et al. 1999 and Chen et al. 2003) to the porous and soft mud seabed. This will provide sediment transport models with more realistic estimates of cross-shore and alongshore velocities in coastal regions with substantial variation in seabed properties. Therefore, improvements in predicting littoral sediment transport will be anticipated. A better prediction of turbidity in coastal regions is of importance to naval deployments of unmanned underwater vehicles (UUV) and divers for inshore countermine warfare. The modeling framework integrated with the CFD Toolkits developed at LSU will allow us to couple the hydrodynamic models with sediment transport models for coastal morphodynamic studies.

In addition to supporting the Navy's research goals, the proposed project will lead to contributions to the Louisiana State University's mission on research and graduate education. A survey conducted by the National Research Council has shown that the north Gulf Coast, where the Naval Research Laboratory and other naval facilities are located, is in need of research and education in coastal engineering. Thus, the proposed training of the post-doctoral fellow and graduate students will enhance the graduate grogram in coastal engineering at LSU to meet the need for graduate education on the Gulf Coast in support of national defense.

TRANSITIONS

None

RELATED PROJECTS

Our project is leveraging and coordinating with activities in several other ongoing activities:

XiRel: This NSF funded project is optimizing and extending an Adaptive Mesh Refinement layer for the Cactus framework, which will be used for our structured grid codes. (http://www.cactuscode.org/Development/xirel)

ALPACA: This NSF funded project is developing debugging and profiling tools for the Cactus framework which will support the Coastal Modeling Framework developed in this project. (http://www.cactuscode.org/Development/alpaca)

CyberTools: This NSF/BOR funded project is developing a cyberinfrastructure across the 100 TFlop machines of the Louisiana Optical Network Initiative. Our project is providing one of the application drivers for this infrastructure. (http://cybertools.loni.org)

CFD IGERT: An NSF graduate training and education program at LSU in training students in computational fluid dynamics and high performance computing. Several research projects are building on the CFD Toolkit which is contributing to our project.

SCOOP: Where appropriate, our models will be integrated into the community infrastructure of the NOAA/ONR funded SURA Coastal Ocean and Observing Program. SCOOP maintains a coastal archive at LSU with realtime forcing and simulation data for storm events.

NSF-CAREER: The five-year research project is focused on simulations of nonlinear coastal waves and air-sea momentum fluxes, which complements the present research project. (http://www.nsf.gov/eng/cbet/nuggets/1443/1443_chen.htm)

The Office of Naval Research new research initiatives of Tidal Flats and Wave-Mud Interactions are closely related to the present study. These provide the project with an excellent opportunity to combine the modeling efforts with the field studies.

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Chen, Q., Tyagi, M., Eksilsson, C. and Allen, G. (2008). Coastal & Ocean Modeling Infrastructure (COMI): Development of an Integrated Modeling Framework for Simulations of Coastal Processes in Deltaic Environments Using High-Performance Computing, CCT Technical Report Series. Louisiana State University.

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